

#Ligand	TotalEnerg	VDW	AverConPa
cav7b3o_NAG-Roccustyrna_fr1-0.pdb	-66.829	-66.829	121.304
cav7b3o_NAG-Roccustyrna_fr2-0.pdb	-916.588	-916.588	184.848
cav7b3o_NAG-Roccustyrna_fr3-0.pdb	254.912	254.912	982.051
cav7b3o_NAG-Roccustyrna_fr4-0.pdb	-699.511	-699.511	145.278
cav7b3o_NAG-Roccustyrna_fr5-0.pdb	433.157	433.157	226.667
cav7b3o_NAG-Roccustyrna_fr6-0.pdb	-836.801	-836.801	141.316
cav7b3o_NAG-Roccustyrna_fr7-0.pdb	-921.261	-921.261	190.571
cav7b3o_NAG-Zanamivir_CID_60855-0.pdb	-760.641	-760.641	21
cav7b3o_NAG-Vidarabine_CID_21704-0.pdb	-748.082	-748.082	231.053
cav7b3o_NAG-Valganciclovir_CID_135413535-0.pdb	440.317	440.317	20.52
cav7b3o_NAG-Tenofovir_CID_464205-0.pdb	-651.681	-651.681	218.421
cav7b3o_NAG-Taribavirin_CID_451448-0.pdb	-683.847	-683.847	242.941
cav7b3o_NAG-Sorivudine_CID_5282192-0.pdb	827.878	827.878	18.2
cav7b3o_NAG-Sofosbuvir_CID_45375808-0.pdb	365.728	365.728	24.25
cav7b3o_NAG-Ritonavir_CID_392622-0.pdb	187.185	187.185	14.12
cav7b3o_NAG-Penciclovir_CID_135398748-0.pdb	-701.763	-701.763	23.5
cav7b3o_NAG-Nelfinavir_CID_64143-0.pdb	416.592	416.592	21.475
cav7b3o_NAG-Merimepodib_CID_153241-0.pdb	-906.535	-906.535	224.242
cav7b3o_NAG-Maribavir_CID_471161-0.pdb	-773.868	-773.868	195.417
cav7b3o_NAG-Lopinavir_CID_92727-0.pdb	405.558	405.558	14.087
cav7b3o_NAG-Indinavir_CID_5362440-0.pdb	-877.687	-877.687	132.889
cav7b3o_NAG-Inarigivir_CID_6912016-0.pdb	-899.455	-899.455	173.333
cav7b3o_NAG-Galidesivir_CID_10445549-0.pdb	-71.061	-71.061	224.211
cav7b3o_NAG-Famciclovir_CID_3324-0.pdb	931.425	931.425	207.391
cav7b3o_NAG-Faldaprevir_CID_42601552-0.pdb	249.487	249.487	151.053
cav7b3o_NAG-Darunavir_CID_213039-0.pdb	-782.833	-782.833	142.632
cav7b3o_NAG-Cytarabine_CID_6253-0.pdb	-672.819	-672.819	234.706
cav7b3o_NAG-Boceprevir_CID_10324367-0.pdb	743.783	743.783	174.324
cav7b3o_NAG-Atazanavir_CID_148192-0.pdb	109.706	109.706	101.569
cav7b3o_NAG-Asunaprevir_CID_16076883-0.pdb	-84.684	-84.684	12.902
cav7b3o_NAG-Amprenavir_CID_65016-0.pdb	-968.745	-968.745	210.571
cav7b3o_NAG-GissitorviffirnaTM1-0.pdb	-750.669	-750.669	213.182
cav7b3o_NAG-GissitorviffirnaTM4-0.pdb	-722.111	-722.111	22.05
cav7b3o_NAG-GissitorviffirnaTM6-0.pdb	405.563	405.563	101.795
cav7b3o_NAG-GissitorviffirnaTM7-0.pdb	-836.518	-836.518	140.526
cav7b3o_NAG-GissitorviffirnaTM8-0.pdb	-956.717	-956.717	169.474
cav7b3o_NAG-GissitorviffirnaTM9-0.pdb	-926.811	-926.811	206.471
cav7b3o_NAG-Roccustyrna_gs1-0.pdb	142.473	142.473	183.043
cav7b3o_NAG-Roccustyrna_gs2-0.pdb	-722.258	-722.258	25
cav7b3o_NAG-Roccustyrna_gs3-0.pdb	235.026	235.026	116.809
cav7b3o_NAG-Roccustyrna_gs4-0.pdb	-158.093	-158.093	132.745
cav7b3o_NAG-Roccustyrna_gs5-0.pdb	375.218	375.218	151.875
cav7b3o_NAG-Roccustyrna_gs6-0.pdb	-67.403	-67.403	22.35
cav7b3o_NAG-Roccustyrna_gs8-0.pdb	747.658	747.658	18.34

